https://doi.org/10.61092/iaea.nnnn-xhex

INDC(NDS)-0908
Distr. G,IBA,IN,J,NM

INDC International Nuclear Data Committee

International Nuclear Data Evaluation Network (INDEN) on the Evaluation of Light Elements (6)

Summary Report of the IAEA Consultants' Meeting

IAEA Headquarters, Vienna, Austria
18 – 22 November 2024

Prepared by

R.J. deBoer
University of Notre Dame
Notre Dame, IN, USA

Marco Pigni
Oak Ridge National Laboratory
Oak Ridge, TN, USA

P. Dimitriou
International Atomic Energy Agency
Vienna, Austria

May 2025

IAEA Nuclear Data Section
Vienna International Centre, P.O. Box 100, 1400 Vienna, Austria

INDC documents may be downloaded in electronic form from

http://nds.iaea.org/publications.

Requests for hardcopy or e-mail transmittal should be directed to

NDS.Contact-Point@iaea.org

or to:

Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre
PO Box 100
1400 Vienna
Austria

INDC(NDS)-0908
Distr. G,IBA,IN,J,NM

International Nuclear Data Evaluation Network (INDEN) on the Evaluation of Light Elements (6)

Summary Report of the IAEA Consultants' Meeting

IAEA Headquarters, Vienna, Austria
18 – 22 November 2024

Prepared by

R.J. deBoer
University of Notre Dame
Notre Dame, IN, USA

Marco Pigni
Oak Ridge National Laboratory
Oak Ridge, TN, USA

P. Dimitriou
International Atomic Energy Agency
Vienna, Austria

ABSTRACT

The INDEN for Light Elements network (INDEN-LE) held a Consultants' Meeting from 18 to 22 November 2024, to review the status of the evaluations undertaken by the Network as well as developments in R-matrix theory and new measurements, and make advancements in the joint evaluation of the ^{7}Be compound system. The summaries of the presentations and discussions can be found in this report.

May 2025

Contents

1. INTRODUCTION

The International Nuclear Data Evaluation Network on the evaluation of Light Elements (INDEN-LE) focuses on evaluating charged-particle- and neutron-induced reactions in the resolved resonance region for light composite systems that are important in energy and non-energy applications. The work carried out by the INDEN-LE has been discussed and documented in the following reports:

Charged particle-induced reactions:

IAEA report INDC(NDS)-0703, 2016: (https://www-nds.iaea.org/publications/indc/indc-nds-0703/)
IAEA report INDC(NDS)-0726, 2017: (https://www-nds.iaea.org/publications/indc/indc-nds-0726/)
IAEA report INDC(NDS)-0737, 2017: (https://www-nds.iaea.org/publications/indc/indc-nds-0737/)
IAEA report INDC(NDS)-0767, 2018: (https://www-nds.iaea.org/publications/indc/indc-nds-0767/)
IAEA report INDC(NDS)-0787, 2019: (https://www-nds.iaea.org/publications/indc/indc-nds-0787/)
IAEA report INDC(NDS)-0827, 2021: (https://www-nds.iaea.org/publications/indc/indc-nds-0827/)

Neutron-induced reactions:

IAEA report INDC(NDS)-0788, 2019: (https://www-nds.iaea.org/publications/indc/indc-nds-0788/)
IAEA report INDC(NDS)-0827, 2021: (https://www-nds.iaea.org/publications/indc/indc-nds-0827/)

Joint reports:

IAEA report INDC(NDS)-0853, 2023: (https://www-nds.iaea.org/publications/indc/indc-nds-0853/)
IAEA report INDC(NDS)-0885, 2024: (https://www-nds.iaea.org/publications/indc/indc-nds-0885/)

The 6th INDEN-LE meeting combined both the R-matrix codes and the neutron-induced reactions and was held from 18 to 22 November 2024, at the IAEA Headquarters, Vienna. The meeting was hybrid and was attended by experts from Austria, China, France, Italy, USA and international organizations.

The IAEA Scientific Secretary, P. Dimitriou, opened the meeting setting out the goals of this meeting and presenting the agenda that comprised morning exercises focused on the evaluation of the ^{7}Be compound system and participants' presentations in the afternoon. The hybrid format in the afternoon allowed for presentations from and discussions with both in-person and remote participants from different time zones. Helmut Leeb was elected chair of the meeting and James deBoer and Marco Pigni were elected rapporteurs.

The summaries of the presentations are given in Section 2, while summaries of the technical discussions and recommendations are provided in Section 3 and the conclusions in Section 4. The adopted Agenda and List of participants are given in Annexes 1 and 2, respectively. Links to participants' presentations can be found at: https://conferences.iaea.org/event/400/

2. PRESENTATION SUMMARIES

2.1. Systematic evaluation of ^{7}Be using Reduced R-matrix Theory and covariance matrices, Z. Chen (Tsinghua University)

In collaboration with Jie Liu and Han Xu

We briefly presented the evaluation results of ^{7}Be, which focus on how to make an evaluation database file for elastic scattering of charged particles including the differential cross sections and their corresponding covariance matrices.

Recently we have developed a more accurate way to publish the covariance matrix of the differential cross section of charged particles by fitting the correlation coefficients, which reduces the size of the file by about 8 times. Each element in the correlation coefficient matrix depends on both energy and angle, so the overall distribution can be analyzed in two approaches. One approach is the energy-dependent distribution at a fixed angle, as shown by the blue part in Fig. 1. The other is the angle-dependent distribution at a fixed energy, as shown by the red part in Fig. 1. which is the approach adopted in this work. The angular distribution of correlation coefficients is smoother and more regular than the energy distribution.

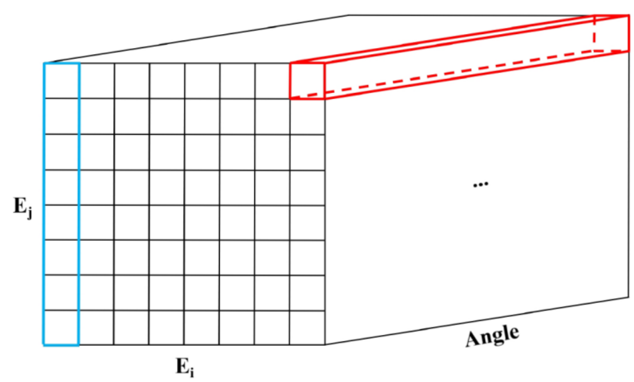

FIG. 1. Schematic diagram of the correlation coefficient matrix.

After obtaining the best set of parameters for R-matrix Analysis (RAC), various types of covariances, including those of various differential cross sections, can be precisely calculated. The advantage of publishing these covariance data in the form of a list is that it is very intuitive, and the disadvantage is that the document volume of the differential cross section covariance of charged particles is particularly large. It is found that the document volume can be greatly reduced by using the correlation coefficient to publish the covariance of the differential cross section of charged particles. For example, for the differential cross section of ^{6}Li (p,p) ^{6}Li, considering 150 nodes from 0.1 to 15MeV in steps of 0.1MeV, the correlation energy pair is (150+1) *150/2=11325. Considering 180 nodes in a step of 1 degree, there are 180 angles in total. If the covariance data is listed in a table a total of 11325*180=2038500 data entries need to be published in the file. The correlation coefficient calculation results show that the angular distribution of each energy pair is a smooth change curve (see Figs 1 and 2), which can be accurately described by a linear background plus several resonances. Since the diagonal of the correlation coefficient matrix consists entirely of ones, we can remove the 150 angular distributions of correlation coefficients corresponding to the diagonal elements of the 150 correlation coefficient matrices. For the remaining 11175 angular distributions, we added a total of 74313 resonances. In addition, each angular distribution requires three background parameters, resulting in a total of (74313+3)*11175=256464 parameter entries. The standard deviation data required for each angle amounts to 180*150=27000 entries. The total number of valid data entries to be published in the file is 256464+27000=259164. Compared to directly providing covariance data, using the format that provides the angular distribution parameters of correlation coefficients to publish data requires approximately 12.7% of the data size compared to directly publishing the covariance data. This means that the volume of the covariance document of the differential cross section of charged particles can be reduced by 8 times. This type of covariance matrix is very fine and does not need to be interpolated when actually called to use. Having addressed this issue, we are ready to publish the results of the light nuclear systematic review, ranging from A= 2 to A=17.

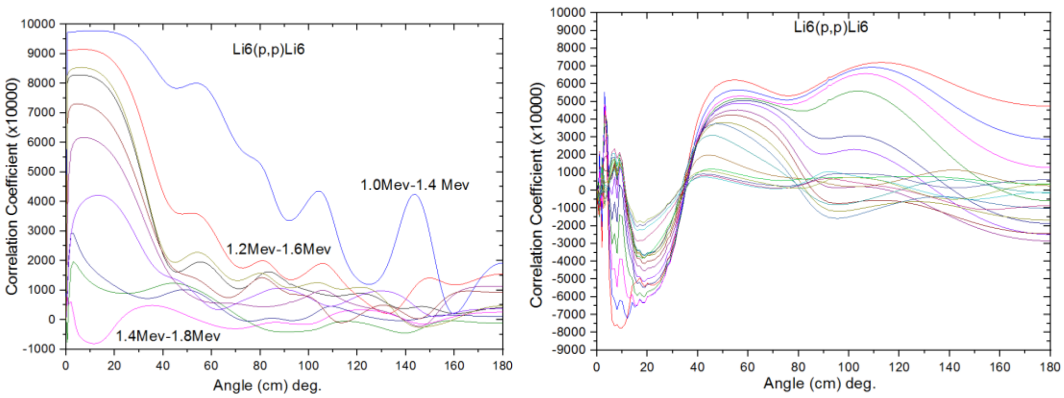

FIG. 2. Angular distribution with respect to non-adjacent energy pairs.

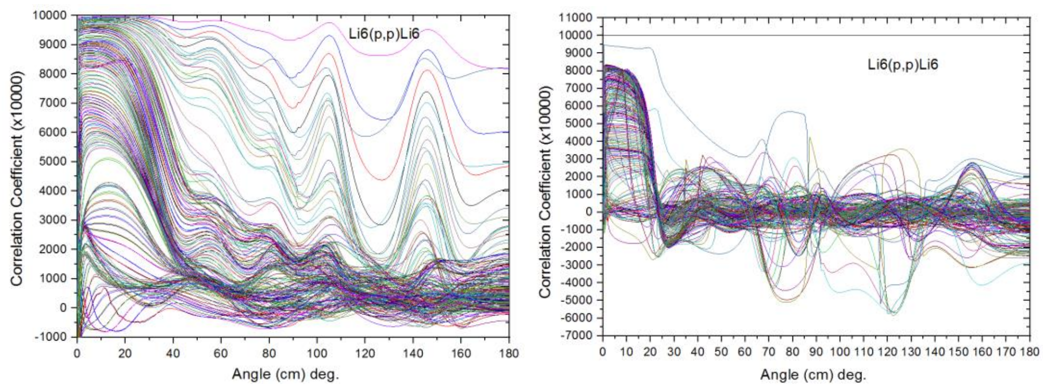

FIG. 3. Same as Fig. 1.

Discussion:

- It would be helpful to see the level diagram that was used in the evaluation, or the energies and spin-parities of the contributing resonances indicated on some of the excitation curve plots.
- The data of Scafes et al. (Eur. Phys. J. A 59:47 (2023)), was added, which overlaps well with Fasoli et al. (Il Nuovo Cimento 34(6), 1832 (1964)) but shows more scatter.

2.2. Application of calculations in the ^{7}Be system and further progress with the ^{17}O system, R.J. deBoer (University of Notre Dame)

In this talk I discussed several projects related to INDEN-LE evaluation work. The first topic was on a recently funded project to measure (α,n) reactions on ^{7}Li, ^{10}B, ^{11}B, ^{13}C and ^{19}F covering the laboratory alpha particle beam energy range from 2 to 8 MeV. These measurements will focus on measuring differential partial cross sections using a novel neutron detector technique that utilizes deuterated liquid scintillators and spectrum unfolding to achieve neutron spectroscopy without time of flight. In addition, we will measure γ-rays and charged particles related to other decay channels, to get as much data as possible to better constrain the subsequent R-matrix evaluations. This experimental campaign will run through 2028.

I summarized my best fit for the ^{7}Be system, where I have been able to obtain a good fit to a representative subset of the data up to an excitation energy of 9 MeV in the ^{3}He+^{4}He and up to 11.6 MeV in the ^{6}Li+p partitions. Above 9 MeV in the ^{3}He(α,α) scattering, I am having a very hard time reproducing the data of Spiger. Unfortunately, there are few other data sets available to provide more information. This has been a major roadblock for a long time. As a related project, Paresh Prajapati and I used this fit as a baseline to show that a proposed (1/2,3/2)+ state near the proton separation energy is highly unlikely, at least with any significant alpha-particle partial width.

While I have not been working on it directly lately, there is a collaboration that is working on an updated evaluation of the low energy ^{13}C(α,n)^{16}O reaction for the ^{17}O system. This is motivated by the recent measurements from LUNA, JUNA, and Notre Dame. Xiaodong Tang's graduate student is currently leading the effort and when I visited them in September they had made a lot of good progress, seemingly essentially done with the project. One additional thing they are pursuing is to see if they can get an estimate of the alpha particle ANC for an additional subthreshold state in ^{17}O, which we think could also contribute to the low energy fit. One big project that I hope to start on soon is extending the R-matrix fit up to the higher energy ranges that we previously measured at Notre Dame. I've only fit the data up to about 3.3 MeV, but it goes up as high as 9 MeV.

I'm trying to complete a couple of analysis for the ^{15}N system. I still have ^{11}B(α,n) and (α,p) from ND that are unpublished. However, Gerry Hale has obtained a good fit to these data and I'm interested to understand how, as I have really struggled with the (α,n) part of the fit. In addition, I'm working on the analysis of new ^{14}N+n total cross section data measured at ELBE at HZDR. The main hang up now is the implementation of energy dependent convolution to model the effects of time-of-flight resolution. The main thing we observed was a smaller peak height for the lowest energy resonance, but it is unclear how this is possible.

2.3. Evaluation of n+^{35,37}Cl, M. Pigni (Oak Ridge National Laboratory)

Performed with support from the U.S. Nuclear Criticality Safety Program to provide improved chlorine cross section and corresponding covariance data, the R-matrix analysis of neutron induced reactions for two stable chlorine isotopes, ^{35,37}Cl, was performed in the energy range of thermal up to 1.2 MeV.

Starting from the repository of the ENDF/B-VIII.0 library and following recent measurement campaigns, this work represents a significant improvement in the evaluation of the (n,p) reaction channel. The evaluation methodology uses the R-matrix code SAMMY to generate a set of Reich-Moore resonance parameters. As predicted by recently measured ^{35}Cl(n,p) data, the presented evaluation features a dramatic increase in the magnitude of the (n,p) reaction channel over the ENDF/B-VIII.0 and previous nuclear data ENDF/B released libraries. Together with details of the evaluation procedure, the impact of the updates in the outgoing proton emissions on reactivity coefficients for one criticality safety benchmark and two molten-salt reactor designs is presented. This shows the impact of the evaluation in the low-energy region up to 1.2 MeV and above that.

2.4. Review of experimental parameter marginalization methods for the production of covariance matrices, P. Tamagno (CEA Cadarache)

Evaluating nuclear data consists in determining not only values for the quantities of interest but also related covariance data. When adjusting nuclear model parameters from experimental data, the covariance matrices are obtained from the propagation of nuclear model parameter uncertainties to nuclear data. When dealing with a model with a small number of parameters compared to the number of experimental data points – e.g. in resonance analysis – one sometimes faces excessively small final uncertainties compared with remaining discrepancies between theory and experiment. To solve this issue a long-standing idea has consisted in transferring the uncertainty of experimental parameters θ involved in the data reduction process on the model parameters x with marginalization techniques.

A simple toy model is introduced to illustrate the marginalization techniques considered here. The model consists of a constant value x with a single "nuisance" parameter θ introduced to account for a possible effect of a state parameter E. To generate a model defect, the experimental data are sampled so that there is no possibility for the toy model to reproduce the data. These latter spreads about two values ±1 (with equal probability) and with small statistical dispersion ±0.1. One therefore expects x=0 and θ=0 for the final values.

Two of the pragmatic marginalization methods often used for evaluation are discussed and some inconsistencies are showed. The first method often called "analytical" aims at finding a marginalized covariance matrix M_p^x on the x parameters alone that yields the same covariance matrix on the evaluated nuclear data as the one obtained when propagating the covariance matrix M_p related to p={θ,x}. This method is shown to be mathematically wrong although some pragmatic "recipes" allow for recovering the desired large uncertainty band on produced data.

A second common marginalization method called here "Bayesian" is also presented; it is shown to produce a large uncertainty with no ad-hoc alteration. However, when applied to the toy model case, it is shown to yield wrong final values for θ as it remains constant in this method. The origin of this default (which may yield Peel's Pertinent Puzzle) is pinpointed in the derivation of the method.

A third method is then presented, it relies on the preservation of the eigenvectors Q of the posterior covariance matrix $M_x = Q\Lambda Q^t$. The marginalized covariance matrix M_x^m on x is defined by the same form but with original eigenvalues Λ_i replaced by Λ_i^m. Several choices are possible to match different criteria. The problem of determining Λ_i^m can be turned into the form of a minimization under constraints. The constraint $\Lambda_i^m \geq \Lambda_i$ ensures that the (first-order) propagated uncertainty for any observable depending on x will be larger than the one obtained by propagation of M_x. Other constraints can be further added in order to tackle the problem of model defect. Two of such constraints are proposed, one (called local) enforcing that all experimental data point lay within a "1σ cumulative uncertainty band", corresponding to the quadratic sum of the experimental uncertainty and the posterior (marginalized) theoretical uncertainty. The second constraint (called global) assumes that all remaining differences between experimental and theoretical values should be Gaussian-distributed and as such defined a global criteria allowing for some points to lie outside the “1σ cumulative uncertainty band”.

This method is illustrated on the toy model and shows to yield the expected final mean values for x and θ, but also a posterior uncertainty band that cover the gap between experimental and theoretical values. The method is then applied on a realistic adjustment of resonance parameters in case of a known model defect. It yields a propagated uncertainty about 50% larger than in the usual Bayesian procedure.

2.5. Uncertainty estimation for R-matrix – J. Skowronski (University of Padua)

Accurate uncertainty quantification in extrapolations of nuclear reaction cross sections is essential for reliable modeling of stellar nucleosynthesis and evolution. In this context, the $^{12}C(p,\gamma)^{13}N$ reaction, a key process in the CNO cycle, was used as benchmark for different uncertainty estimation approaches. Experimental cross-section data for this reaction exhibit significant discrepancies, which necessitates a robust methodology for R-matrix fitting and uncertainty estimation.

Four distinct uncertainty estimation methods were applied to R-matrix fits of the ^{13}N compound. The first approach is a frequentist chi-squared minimization, which relies on the covariance matrix calculation. This method suffered from underestimation of uncertainties and the presence of local minima, which resulted in locally converging fits depending on the initial parameter values. The covariance matrix frequently was poorly conditioned, leading to narrow confidence intervals that failed to capture the full range of possible solutions. To address these limitations, a hybrid frequentist approach was shown as well. This method samples dataset normalization factors from log-normal distributions based on their systematic uncertainties, treating them as random variables rather than fixed parameters. By conducting parallel minimizations with varying normalizations, the hybrid method reduces sensitivity to local minima and produces a broader, more realistic uncertainty band. This approach successfully mitigates the covariance matrix issue by decoupling parameter uncertainties from the dataset normalizations and thus offers a more robust estimation of the total uncertainty.

The third method was the Bayesian inference using a standard Markov Chain Monte Carlo (MCMC) algorithm to sample the posterior distribution of the R-matrix parameters. While the Bayesian approach provides a natural framework for parameter estimation, it was too limited by the presence of multiple local minima in the parameter space, causing the MCMC sampler to become trapped and under-sampling the full distribution. This led to underestimated uncertainties, particularly in cases where datasets exhibit significant discrepancies. To overcome the limitations of standard MCMC, a tempered MCMC Bayesian method was shown. This technique introduces temperature parameters, allowing the sampler to traverse probability barriers between local minima and explore the parameter space more comprehensively. By running multiple parallel chains with varying acceptance criteria and periodically exchanging information between them, the tempered MCMC approach effectively samples the full posterior distribution, capturing the multi-modal nature of the parameter space. The resulting uncertainty estimates are broader and more reflective of the true variability in the cross-section data.

Comparison of the four methods reveals significant differences in uncertainty estimation. The classic frequentist and Bayesian approaches underestimates uncertainties due to the local minima in the parameter space, while the hybrid frequentist and tempered MCMC methods provide more consistent and reliable uncertainty bands. These findings highlight the importance of using advanced statistical techniques in R-matrix analyses to ensure robust and reproducible uncertainty quantification, particularly for nuclear reactions with astrophysical relevance.

Discussion:

- Comment and question: similar solutions can be found with both the "minimization" and Bayesian approaches if both approaches have probability distributions close to normal or gaussian distributions. The frequentist approach is something quite different. In this case, it is almost as if one is looking at the probability distribution function of data as if one could perform experiments infinitely many times. Then, one could make statements about the nature of that probability distribution function rather than fit the parameters to some given model. To summarize, the posterior has different forms depending on the assumptions about the probability functions. Therefore, the chi-squared and MCMC approaches could be viewed as both falling within the Bayesian optimization techniques?
- Comment: In reply to the above question, I have an analytical example, where you compare sampling and chi-squared minimization. This study has essentially been done in the context of polynomial fitting by Matthias Schindler and Daniel Phillips in M.R. Schindler and D.R. Phillips, Annals of Physics 324 (2009) 682.
- Comment on the PTMC which is a great tool for multimodal distributions, even in some cases where the distribution is not multimodal. The concept of temperature is rigorously defined since what one is doing is creating chains that have different mixes of the prior and likelihood. At infinite temperature, it is all prior and no likelihood. At temperature equals 1, one is sampling the target distribution which is the likelihood times the prior. These different chains basically have different amounts of likelihood in them and therefore have different depths of wells into which one can fall into. So, if the concept of temperature is rigorously defined, one can prove that detailed balance works if one implements the temperature swaps carefully. One has the same theorems that guarantee convergence in the case of the standard Markov chain Monte Carlo.

2.6. BRICK and Beyond: Bayesian analyses of low-energy ^{3}He-^{4}He data using R-matrix and Effective Field Theory, D.R. Phillips (Ohio University)

A new set of low-energy data on the elastic ^{3}He-^{4}He scattering reaction was published earlier this year [1]. It consists of 451 measurements at nine beam energies ranging from 0.721-5.490 MeV and has well documented & constrained systematic uncertainties. It was obtained at TRIUMF by impinging a ^{3}He beam on the SONIK apparatus filled with ^{4}He gas. This is the only measurement of this reaction at the center-of-mass energies below 500 keV.

In Ref. [2] the Bayesian R-matrix Inference Code Kit (BRICK) was used to perform a Bayesian calibration of an R-matrix model. The calibration included these SONIK data, together with 88 S-factor data on the radiative capture reaction ^{3}He(α,γ) below 3.0 MeV, and 646 data from the elastic scattering data set of Barnard [3]. The R-matrix model included the 3/2- and 1/2- bound states of ^{7}Be, together with resonances with Jπ=5/2- and 7/2-, and background resonances in several other channels.

BRICK couples a Markov Chain Monte Carlo sampling tool to AZURE2 and is part of the publicly available BAND software framework [4]. It provides

- Access to the full, correlated, multi-dimensional posterior for the parameters of the R-matrix model. This permits diagnosis of multi-modality allowing one to see if posteriors are non-Gaussian, and reveals which parameters are not influenced by the likelihood.
- Any observable of interest can be evaluated from the samples of the R-matrix parameters drawn from the posterior. Error propagation—even beyond the linear approximation—is then straightforward.
- "Nuisance parameters" can be introduced to model experimental imperfections. Marginalizing over those parameters includes the imperfections' impact on parameters and evaluated quantities. In Ref. [1] nuisance parameters were introduced to treat acceptance effects at specific (lab.) angles and Ref. [2] used them to account for beam-energy shifts. The analyses of Refs. [1,2] also both considered common-mode errors for all data sets.

The SONIK and capture data are simultaneously well reproduced in the fits of Refs. [1,2]. However, the R-matrix model can only reconcile the capture data of Ref. [5] with the Barnard scattering data if a large normalization factor is applied to it. This is ultimately because there is tension between the ^{7}Be Asymptotic Normalization Coefficients inferred from the scattering data of Ref. [3] and those inferred from the radiative capture data.

The Halo Effective Field Theory has also been used to analyse the same set of capture data and the data of Ref. [1]. It provides a good fit to the S-factor [6] and to scattering data below the 7/2- resonance [7]. But the s-wave scattering length deduced in Halo EFT is systematically larger than that found in R-matrix analyses.

This work was supported by the U.S. Department of Energy, National Nuclear Security Administration under Award DE- NA0003883, and Office of Science, Office of Nuclear Physics, under Award DE-FG02-93ER-40756, as well as by the National Science Foundation under grant OAC-2004601 (CSSI program, BAND collaboration).

References

[1] S. N. Paneru et al., Phys. Rev. C **109** (2024) 015802.
[2] D. Odell, C. R. Brune, D. R. Phillips, R. J. deBoer, and S. N. Paneru, Front. Phys. **10**:888476 (2022).
[3] A. Barnard, C. Jones, and G. Phillips, Nucl. Phys. **50** (1964) 629.
[4] https://github.com/odell/brick, see also https://bandframework.github.io/.
[5] Costantini H et al., Nucl. Phys A **814** (2008) 144.
[6] X. Zhang, K. M. Nollett, and D. R. Phillips, J. Phys. G **47** (2020) 054002.
[7] M. Poudel and D. R. Phillips, J. Phys. G **49** (2022) 045102.

Discussion:

- Question: How do you deal with the beam energy shift in your analysis?
  Answer: It is a parameter that is calibrated using MCMC sampling in the same way as other parameters of the fit. In the case of ^{3}He-alpha elastic scattering it seems the Barnard data need to be shifted in energy by about 20 keV. This is, though, within the uncertainty in the energy quoted in the Barnard et al. publication.
- Question: But then the external capture integral depends on the energy of the data points. So how do you deal with energy shifts in that case?
  Answer: in BRICK the external capture integrals are indeed recalculated each time AZURE2 is used to evaluate the cross section at a new set of parameter values. This makes it very

computationally expensive to calibrate beam energy shifts for capture data. The analyses described in this presentation only considered beam energy shifts for experiments that measured elastic scattering cross sections. A more efficient use of AZURE2 (e.g. computing only once all pieces of the calculation that are not dependent on the R-matrix parameters) should be developed in future work.

2.7. R-matrix analysis of ^{8}Be system, S.N. Paneru (Los Alamos National Laboratory)

Charged particle-induced reactions on light nuclei are important for both nuclear applications and nuclear astrophysics. These reactions are typically studied using R-matrix analysis to determine the best estimates of their cross sections and quantify uncertainties, which are then reported to data libraries like ENDF.

Discrepancies and inconsistencies among various data libraries for reactions forming a compound ^{8}Be system have been identified. The evaluation reported to the ENDF/B-VIII.1 library for the ^{8}Be system is incomplete, as the R-matrix analysis used for this evaluation did not include data for reactions resulting in the residual nucleus being in excited states, such as ^{6}Li(d,n$_1$)^{7}Be, ^{7}Li(p,n$_1$)^{7}Be, etc.

To improve the evaluation of ^{8}Be, a new, comprehensive R-matrix analysis was performed, incorporating data for all reaction channels. This analysis included additional data from a recent, comprehensive measurement of deuterium-induced reactions on ^{6}Li. The experiment simultaneously measured all outgoing reaction products—neutrons, charged particles, and gammas. Notably, the partial cross sections for ^{6}Li(d,n$_0$)^{7}Be and ^{6}Li(d,n$_1$)^{7}Be up to deuteron energies of 10 MeV were reported from this measurement for the first time.

The R-matrix analysis was performed using the phenomenological R-matrix code AZURE2. Uncertainties in the R-matrix parameters and cross sections were inferred using the Bayesian R-matrix Inference Code Kit (BRICK). Altogether, more than 2,500 data points were fitted simultaneously, achieving a reasonable fit across all channels.

This analysis highlighted the incompleteness of the ENDF/B-VIII.1 library. The lessons learned are already being applied to the ^{8}Be evaluation using the Energy Dependent Analysis (EDA) R-matrix code at Los Alamos National Laboratory. The results from the improved EDA evaluation of the ^{8}Be system will be reported to the ENDF/B-IX library.

Discussion:

- Question: Do you know which channels have been neglected?
  Answer: At higher energies some excited state channels may have been neglected. Also, multiparticle breakup is neglected, which is also energetically possible (e.g. $\alpha+\alpha+\alpha$).
- Question: What is the minimization technique in EDA?
  Answer: It is a frequentist technique.

2.8. Progress in evaluation of n+^{9}Be, H. Leeb (Technische Universität Wien)

The focus of the nuclear data group at TU Wien is the development of a Bayesian-based evaluation technique for neutron-induced reactions of light nuclear systems, e.g. ^{6,7}Li, ^{9}Be, ^{12}C and ^{16}O. In the present contribution the current status of the n+^{9}Be evaluation, performed at TU Wien, was presented. The retrieval and examination of available experimental data sets included angle-integrated data, angle-differential data and excitation functions for incident neutron energies up to 30 MeV. The n+^{9}Be system involves the four-body breakup ^{9}Be(n,2nα)^{4}He with very low threshold energy corresponding to Q = -1.6636 MeV. The breakup channel cannot be included in a standard R-matrix analysis. Therefore, a Reduced R-matrix analysis with the code GECCCOS [1] was performed considering the breakup channel as an ignored one. The implemented Reduced R-matrix approach differs from the Reich-Moore approximation and is also different to that of RAC. The method in GECCCOS allows an imaginary part of the R-matrix only at energies above the threshold of the breakup channel. A first R-matrix analysis was limited to incident neutron energies up to 10 MeV which included besides the elastic scattering only two inelastic channels, the ^{9}Be(n,α)^{6}He reaction, the total cross section and as ignored channel the breakup reaction. This first R-matrix analysis provided an excellent description of the experimental data, both integrated as well as differential ones. Extending the energy range of the Reduced R-matrix analysis to incident neutron energies up to 30 MeV required the inclusion of further channels, e.g. the (n,t)-reaction, and additional sets of experimental data. Unfortunately, despite numerous searches, a satisfactory Reduced R-matrix description of all channels could not be achieved. Especially, the breakup- and the (n,α)-channel were badly reproduced. A comparison of the results indicated that the main problem is related with the description of the strong resonance at E_n~2.7MeV which leads to high values of the corresponding reduced widths and thus to strong correlations in energy. In order to solve the problem, we proposed either R-matrix fits using Brune's [2] or Park's parametrization [3] or to split R-matrix analyses thus effectively suppressing the correlations. However, both proposals require modifications of our codes which are currently in progress.

Furthermore, the inherent problem of an R-matrix-based evaluation was addressed. Performing an R-matrix analysis implies the use of experimental data, and thus the a-priori information required in an Bayesian evaluation technique is still an open problem. A first proposal for the determination of an R-matrix based prior was presented by our group [1]. A genuine a-priori information is provided by the level scheme (E_x, J^{π}) of the compound nucleus and the thresholds of involved channels. Thus, an R-matrix based prior was generated via Monte Carlo sweeps with the R-matrix code GECCCOS varying energies, matching radius and relevant g-widths each in a reasonable range. The variation of the energy was included because the standard R-matrix poles do not coincide with resonance energies. Because of the problems discussed above the energy range of the prior was determined only up to 10 MeV incident neutron energy. The generated prior together with the experimental data were used in a modified general least square fit [4] and yields the evaluated mean values and the covariance matrices of the uncertainties of the cross sections. In the determination of the prior only the relevant γ-widths (not the values) from the R-matrix analysis are varied. Thus, the method is almost independent from experimental data. Currently the implementation to an improved R-matrix analysis and the corresponding implementation in the evaluation code are in progress.

Work partly supported by the Euratom project SANDA (Grant Number No 847552). Views and opinions expressed are however those of the author(s) and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them.

[1] H. Leeb, T. Srdinko, EPJ Web of Conf. **294** (2024) 04006.
[2] C.R. Brune, Phys. Rev. C **66** (2002) 044611.
[3] Tae-Sun Park, Phys. Rev. C **104** (2021) 064612.
[4] G. Schnabel, H. Leeb, Nucl. Inst. Meth. A **841** (2017) 87.

Discussion:

- The transformations by Park and Brune are different. They are equivalent, but unfortunately the parameters are not the same. While it should be possible, there is currently no transformation between the different parameters. It has also been noted that it can be difficult to get an exact transformation between Brune and formal R-matrix parameterizations. Even so, it is close, and the Brune or Park parameterizations provide a much more intuitive way to fit because the pole energies correspond to the resonance energies.
- A question was asked whether a better formulated direct reaction mechanism needs to be included at higher energies to fix the problem of reconciling the low-energy resonance region with the higher-energy statistical regime.

3. Technical discussions

3.1. Test 3 – Full evaluation of ^{7}Be compound system

Revised at INDEN-LE meeting, 18-22 Nov. 2024, IAEA

The conditions for performing a full evaluation of ^{7}Be have been laid out at previous meetings and are mentioned in the corresponding meeting reports (INDC(NDS)-0726, INDC(NDS)-0787, INDC(NDS)-0827). They were revised during discussions held on 01-09-2022. Present: P. Dimitriou, H. Leeb, M. Pigni, I. Thompson, and shared with all participants of the exercises.

Herein, we present a final review of the conditions of the exercise to produce an evaluation of the ^{7}Be system. The end goal is to publish these evaluations in a peer-reviewed journal.

Conditions

1) Three incident channels will be considered according to the experimental data available in EXFOR:

p+^{6}Li, E_x = 11.5 MeV at least ($E_p \approx$ 7 MeV (lab));

^{3}He+^{4}He, E_x = 11.5 MeV at least ($E_{3He} \approx$ 23 MeV (lab));

^{4}He+^{3}He, E_x = 11.5 MeV at least ($E_{4He} \approx$ 17 MeV (lab)).

Ignore gamma and inelastic channels.

2) Experimental data – revised

We use the same datasets adopted by Ian in his ENDF/B-8.1 evaluation below, with the addition of the Ivanovich (α,α) data. The Lin (p,α) will be checked.

The following 10 data sets were included in Ian's ENDF/B-8.1 file –

```
ENDF/B-VIII.1 Evaluation, October 2022,
  I.J. Thompson (LLNL) and INDEN-light-element collaboration
  Candidate evaluation produced with Frescox code

SUMMARY

  This evaluation is the result of R-matrix fits performed
by members of the INDEN Light-element collaboration meeting
at IAEA in combined h+a and p+Li6 modelling.
The capture channel and Li6 excited states are not yet included.

  It uses the B=-L R-matrix boundary conditions,
with maximum partial waves of 4 for h+a and 1 for p+Li6,
and spin groups up to J=9/2.
The channel radii are (1.4 fm) * (A1^1/3 + A2^1/3).
The R-matrix parameters are in MF=2 in LRF=7 KRM=4 IFG=1 format
Elastic Coulomb scattering is given with LTP=2 Legendre terms

Fitted Data:

  Dataset       Chisq/pts  av norm  av E shift (MeV)
  Barnard_aa    0.967      0.990
  Elwyn_pa      4.317      1.133
  Fasoli_pp     3.895      0.996
  Harrison_pp0  5.489      1.156
  Lin_pa        3.885      1.305
  McCray_pp     3.842      1.122
  Mohr_aa       3.481      0.956
  Spiger-aa     2.633      0.929      -0.048
  Spiger-cm_ap0 1.419      1.004
  Tombrello_aa  3.559      1.080      -0.036

Translated via GNDS to ENDF6 by FUDGE.
```

Additional checks:

- The datafiles will be taken from the shared OneDrive folder: Rmatrix_codes/Be-7/ Final_data_2024

  Need to add the Ivanovich data from EXFOR.

  Action: J. deBoer and J. Skowronski will include data from EXFOR as needed to cover the agreed excitation energy range.
- The data are also available in the Rflow GitHub repository – in the CM system.
  Action: on J. Skowronski to check the data in Rflow in comparison with the data in the OneDrive.
- **Action:** WHO? Check I. Thompson's properties tables and normalizations – correct the 3 files with issues if needed (slide 3 of Ian's 2023 presentation)
- Keep the Lin (p,alpha) data in the OneDrive folder.
- SONIK data: provided by Som Paneru (LANL) for ^{3}He+^{4}He. The data are in the CM. Both incident beam and effective energy at 3 interaction regions are provided.
  Action: on J deBoer to review these data and suggest how to use them in the evaluation.
- Also update properties of the data including information on cm/lab, type (ang. distr. or excit. function or shape data), normalizations in data.prop.csv and systematics.csv files.

  Action on J. deBoer and J. Skowronski.
- Consider creating an IAEA Github repository for the project (fork Ian's RMACP repo).
  Action on V. Dimitriou and J. Skowronski to contact I. Thompson about forking the two GitHub repositories.

Note: J. deBoer data files do not contain any metadata (units, type of data, etc.)

Use datafile.props.csv and systematics.csv files for properties and additional information on systematic uncertainties etc from James.

3) Input resonance energies, widths, spins and parities

First step: we reproduce the ENDF/B-8.1 ^{3}He+^{4}He evaluation using the ENDF/B-8.1 resonance parameters (MF=2).

Compare the ENDF/B-8.1 resonance parameter file (MF=2) and cross sections with Rflow and with measured cross sections.

Starting from the ENDF/B-8.1 resonance parameter file which corresponds to E_x = 7.5 MeV of ^{7}Be, add the levels necessary to extend the evaluation to E_x = 11.5 MeV of ^{7}Be.

The ENDF/B-8.1 resonance parameter file is almost identical to Test 2 (with the exception of one background pole used in Test 2). To be converted to AZURE2 (and other) formats with Ferdinand.

Action on J. Skowronski.

4) Output data (to be provided by evaluators) – no changes

- Chi2/dof
- Resonance parameter (RP) files
- Reconstructed cross-section files
- Use Legendre expansions for elastic scattering charged-particle angular distributions - if possible
- Covariances of RP and/or reconstructed cross sections (ENDF6 specifications)
- List of data normalizations
- Experimental data - metadata (whatever modifications have been implemented)

5) Requirement for participation in INDEN evaluation – no changes

To provide all output listed in (4) by agreed deadlines

Actions/Deadlines and Recommendations

- **December 31, 2024:** all code developers who contributed to Test 2 to provide a folder with resonance parameter files and output files (cross sections and covariances on parameters).
- **December 31, 2024**, for all the actions in paragraphs 2 and 3) above and delivery of final exp. database.
- **April 30, 2025**, online meeting: present preliminary evaluations; obtain feedback.
- **September 30, 2025**, final evaluations and all files mentioned in paragraph 4).
- By the next INDEN-LE meeting (Nov. 2025): first draft of the paper (consider Eur. Phys. J. A or Nuclear Data Sheets)
- The ^{7}Be evaluations performed by RAC and EDA codes should be compared with the joint INDEN-LE evaluation.

3.2. Additional action items and recommendations

- The structure data are crucial to any evaluation. This group should maintain close contact with the ENSDF evaluators for feedback on new data or issues in the existing structure data.
- Send lithium cross section data (^{6}Li+d) to Goran Arbanas for sensitivity analysis in integral benchmark experiments – Som Paneru.
- Discuss extending the ^{7}Be evaluations to higher energies after completing the initial evaluations – everyone.
- Consider updating the aluminium evaluation if there are relevant new data sets available - everyone
- Evaluate the channels for scattering and secondary gamma rays and make them available through IBANDL – James deBoer.
- Reach out to other people and see who is working on ^{17}O.
- Investigate the work of Goldberg at Texas A&M University on scattering measurements using R-matrix analysis.
- Reach out to the group in Japan that does elastic and inelastic scattering and alpha-p measurements using R-matrix analysis.
- Inquire about the group in Birmingham, UK that specializes in cluster physics and cluster models to see if they use R-matrix analysis.
- Reach out to Suprita Chakraborty in India to see if she is interested in participating.
- Submit an abstract of the ^{7}Be evaluation to ND2025 – Vivian Dimitriou.

4. Conclusions

The INDEN-LE group met to discuss the progress of the evaluations of ^{7}Be and other ongoing projects relevant to light-element reactions in the resolved resonance region. The conditions for the ^{7}Be evaluation were reviewed and updated and deadlines were fixed. Efforts to reach out to other research groups with overlapping interests were proposed.

It was suggested that after the completion of the evaluation of ^{7}Be, an evaluation of ^{17}O and ^{28}Si should be considered due to their importance in several applications such as reactor operation, ion beam analysis, accelerator and detector calibration, and nuclear astrophysics, and Dark Matter searches. The details of such an evaluation will be discussed at the next INDEN-LE meeting in 2025.

ANNEX 1

IAEA Consultancy Meeting of the International Nuclear Data Evaluation Network – Light Elements

18 – 22 November 2024, IAEA, Vienna
MOE127 (virtual component)

ADOPTED AGENDA

Monday, 18 November

10:00	**Test 3: ^{7}Be evaluation practical session**		*Breaks as needed*
12:00	***Lunch break***		
13:00 – 17:00	**Participants' Presentations**		
	P. Dimitriou	Introduction and goals	
	J. Liu et al.	Systematically evaluate ^{7}Be using reduced R-matrix theory	
	R. deBoer	Application of calculations in the ^{7}Be system and further progress with the ^{17}O system	
	M. Pigni	R-matrix analysis of n+natCl reations relevant to criticality safety benchmarks and molten-salt reactor designs	
	P. Dimitriou	Status report on ^{19}F(alpha,n) and ^{7}Be	
	J. Kelley	Comments on nuclear structure data	

Tuesday, 19 November

10:00	**Test 3: ^{7}Be evaluation practical session**		*Breaks as needed*
12:00	***Lunch break***		
13:30 – 17:00	**Participants' Presentations** cont'		
	P. Tamagno	Review of experimental parameter marginalization methods for the production of covariance matrices	
	J. Skowronski	Uncertainty estimation for R-matrix evaluations	
	D. Phillips	BRICK and beyond: Bayesian analyses of low-energy ^{3}He-^{4}He data using R-matrix and Effective Field Theory	
	S. Paneru	R-matrix analysis of ^{8}Be system	

Dinner at a restaurant (separate information)

Wednesday, 20 November

10:00	**Test 3: ^{7}Be evaluation practical session**	*Breaks as needed*
12:00	***Lunch break***	
13:30 – 17:00	**Roundtable discussion: Future of INDEN-LE and how to proceed**	

Thursday, 21 November

10:00	**Participants' Presentations** cont'		*Breaks as needed*
	H. Leeb	Progress in evaluation of n+^{9}Be	
10:45	**Test 3: ^{7}Be evaluation practical session**		
12:00	***Lunch break***		
13:30 – 17:00	**Discussion & Drafting of the meeting summary report**		

Friday, 22 November

10:00	**Discussion & Drafting of the meeting summary report** cont'	*Break as needed*
13:00	**Closing of the meeting**	

IAEA Consultancy Meeting of the International Nuclear Data Evaluation Network – Light Elements

18 – 22 November 2024, IAEA, Vienna
MOE127 (virtual component)

PARTICIPANTS

Country / Organization		Name	Surname	Affiliation	Email
AUSTRIA		Helmut	LEEB	Technische Universität Wien	helmut.leeb@tuwien.ac.at
		Thomas	SRDINKO	Technische Universität Wien	thomas.srdinko@tuwien.ac.at
CHINA	🎧	Han	XU	Institute of Computational Physics and Computational Mathematics	hanxu22@gscaep.ac.cn
	🎧	Zhenpeng	CHEN	Tsinghua University	zhpchen@tsinghua.edu.cn
FRANCE		Pierre	TAMAGNO	Atomic Energy and Alternative Energies Commission	pierre.tamagno@cea.fr
ITALY		Jakub	SKOWRONSKI	University of Padova, Dept. of Physics and Astronomy	jakub.skowronski@pd.infn.it
USA		Richard J.	DEBOER	University of Notre Dame, Dept. of Physics and Astronomy	Richard.J.deBoer.12@nd.edu
		Marco	PIGNI	Oak Ridge National Laboratory	pignimt@ornl.gov
	🎧	Goran	ARBANAS	Oak Ridge National Laboratory	arbanasg@ornl.gov
	🎧	Carl Richard	BRUNE	Ohio University	brune@ohio.edu
	🎧	Gerald	HALE	Los Alamos National Laboratory	ghale@lanl.gov
	🎧	Daniel	PHILLIPS	Ohio University	phillid1@ohio.edu
	🎧	John	KELLEY	Duke University, Triangle Universities National Laboratory	jhkelley@duke.edu
	🎧	Kiana	SETOODEHNIA	Duke University, Triangle Universities National Laboratory	kiana.setoodehnia@duke.edu
	🎧	Gregorio P.	POTEL AGUILAR	Lawrence Livermore National Laboratory	potelaguilar1@llnl.gov
	🎧	Hye Young	LEE	Los Alamos National Laboratory	hylee@lanl.gov
Int. Organization	🎧	Daniela	FOLIGNO	Nuclear Energy Agency (NEA)	daniela.foligno@oecd-nea.org
		Paraskevi	DIMITRIOU	International Atomic Energy Agency	p.dimitriou@iaea.org

Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre, P.O. Box 100
A-1400 Vienna, Austria

E-mail: nds.contact-point@iaea.org
Fax: (43-1) 26007
Telephone: (43-1) 2600 21725
Web: https://nds.iaea.org